

ABSTRACT

A user inputs target sequence data (10) that is primary sequence information on a target protein to an interaction site prediction apparatus of this invention. A fragment structure prediction simulation is executed to the target sequence data (10) input to each of
5 fragment structure prediction programs (20a to 20d) for predicting a fragment structure of the protein from the primary sequence information on the protein. Fragment structure prediction results (30a to 30d) of the respective fragment structure prediction programs (20a to 20d) are
10 compared with one another (60). Based on this comparison result, a frustration of a local part of the primary sequence information on the target protein is calculated (70). An interaction site in the target protein is predicted based on the calculated frustration of the local part (80).